ABSTRACT

COMPUTER-AIDED METHOD FOR THE PROVISION, IDENTIFICATION AND DESCRIPTION OF MOLECULES CAPABLE OF EXHIBITING A DESIRED BEHAVIOUR, MORE PARTICULARLY IN THE PHARMACEUTICAL SECTOR, AND MOLECULES OBTAINED BY SAID METHOD

The present invention is concerned with a computer-aided method for the provision, identification and description of molecules exhibiting a desired behaviour, more particularly in the pharmaceutical sector, employing a molecular modelling step, a combinatorial library building step and a step of selecting potentially useful molecules, said method including a step whereby the candidate molecules are filtered using a dynamic filter representing constraints of conformational variations which the molecules must satisfy in order to exhibit said activity.